



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:36 pm GMT

PDB ID : 1QW1
Title : Solution Structure of the C-Terminal Domain of DtxR residues 110-226
Authors : Wylie, G.P.; Rangachari, V.; Bienkiewicz, E.A.; Love, J.F.; Murphy, J.R.; Logan, T.M.
Deposited on : 2003-08-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

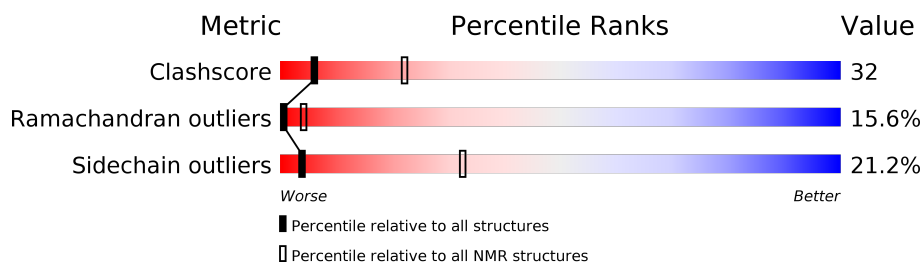
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

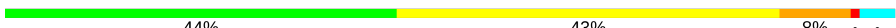
The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	121	

2 Ensemble composition and analysis

This entry contains 14 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:111-A:226 (116)	1.07	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 9, 10, 11, 12, 13, 14
2	7, 8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1874 atoms, of which 938 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Diphtheria toxin repressor.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1874	577	938	168	189	2	

There are 4 discrepancies between the modelled and reference sequences:

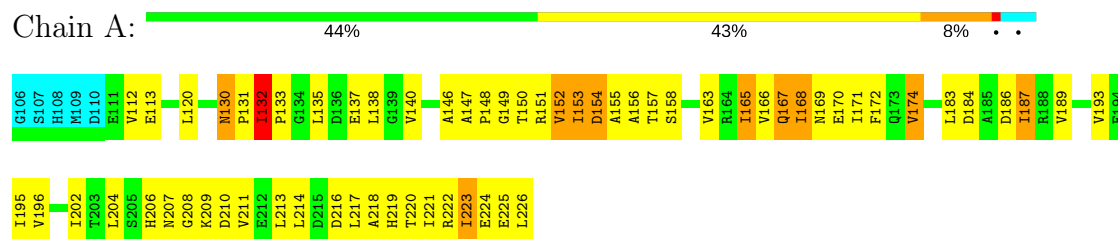
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	CLONING ARTIFACT	UNP P33120
A	107	SER	-	CLONING ARTIFACT	UNP P33120
A	108	HIS	-	CLONING ARTIFACT	UNP P33120
A	109	MET	-	CLONING ARTIFACT	UNP P33120

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Diphtheria toxin repressor

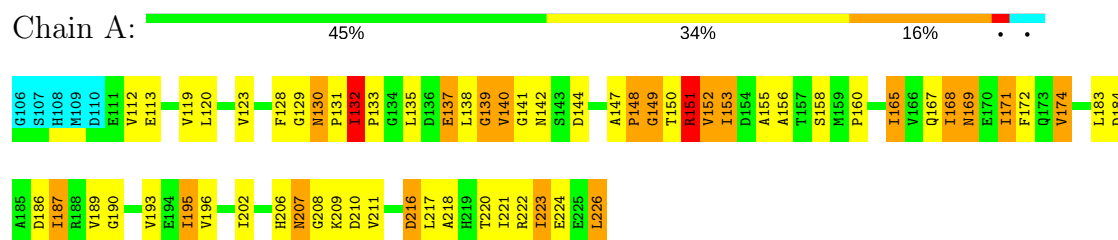


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Diphtheria toxin repressor



4.2.2 Score per residue for model 2

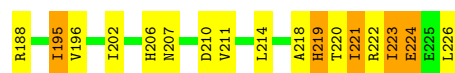
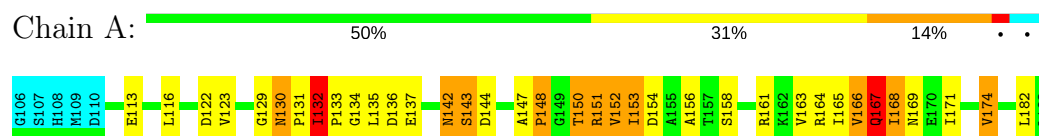
- Molecule 1: Diphtheria toxin repressor





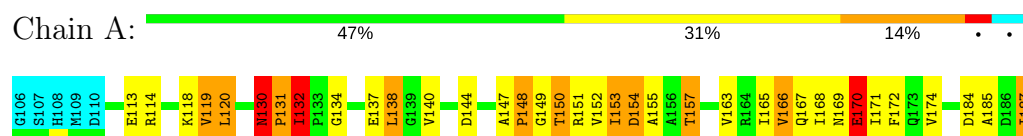
4.2.3 Score per residue for model 3

- Molecule 1: Diphtheria toxin repressor



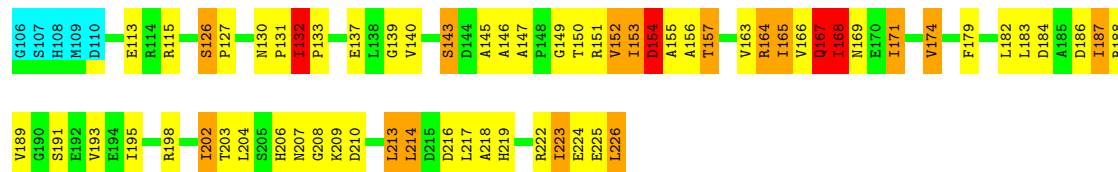
4.2.4 Score per residue for model 4

- Molecule 1: Diphtheria toxin repressor



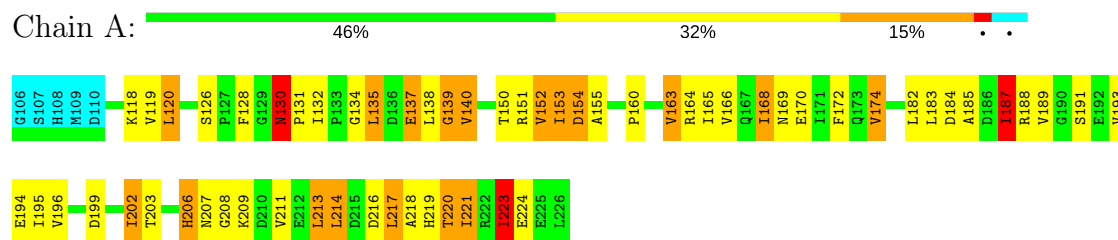
4.2.5 Score per residue for model 5

- Molecule 1: Diphtheria toxin repressor



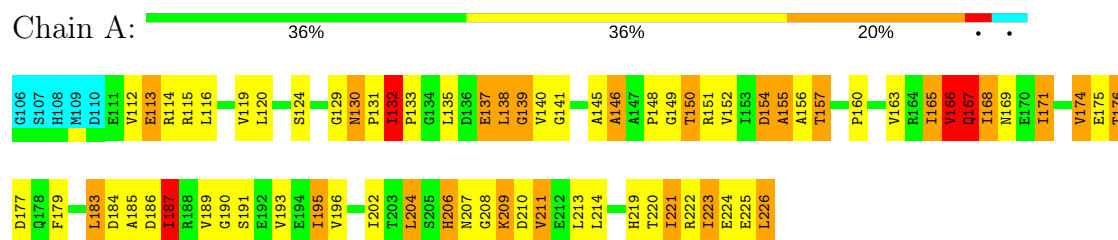
4.2.6 Score per residue for model 6

- Molecule 1: Diphtheria toxin repressor



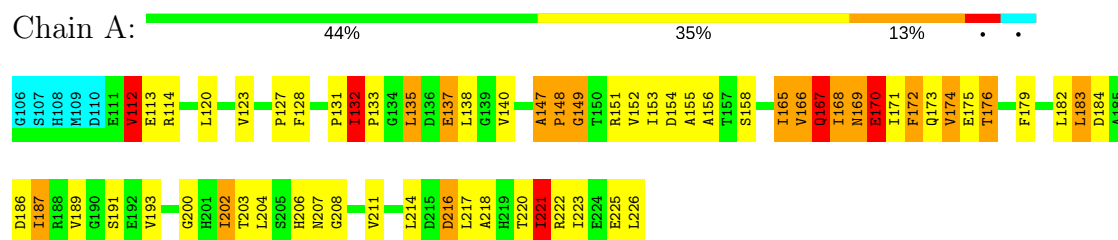
4.2.7 Score per residue for model 7

- Molecule 1: Diphtheria toxin repressor



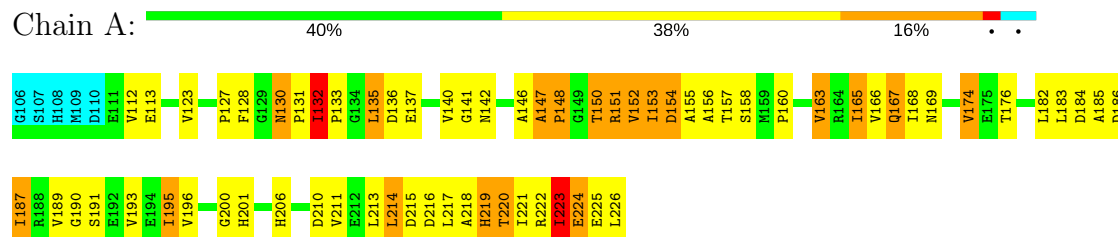
4.2.8 Score per residue for model 8

- Molecule 1: Diphtheria toxin repressor



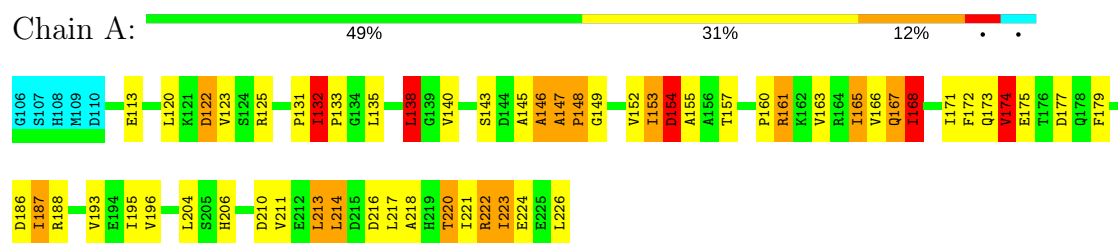
4.2.9 Score per residue for model 9

- Molecule 1: Diphtheria toxin repressor



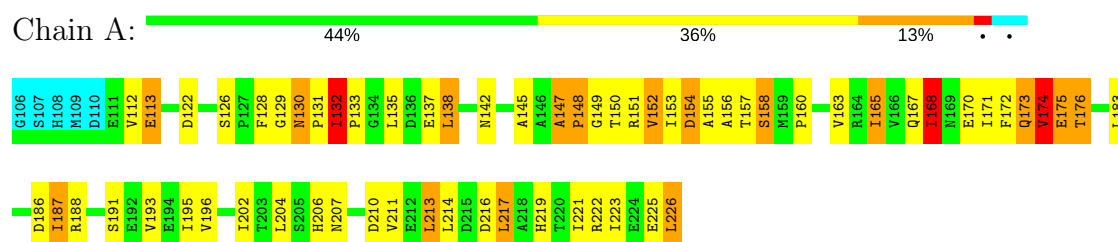
4.2.10 Score per residue for model 10

- Molecule 1: Diphtheria toxin repressor



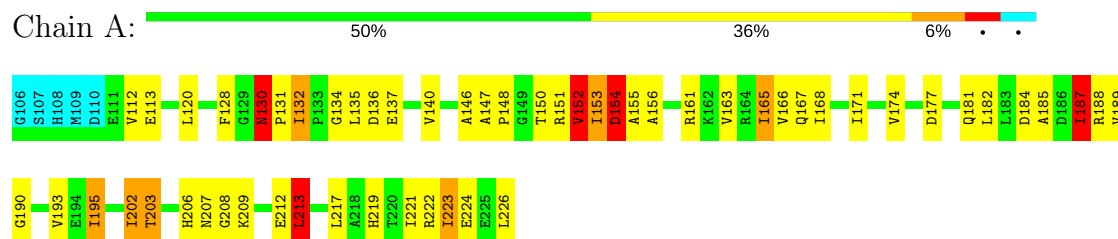
4.2.11 Score per residue for model 11

- Molecule 1: Diphtheria toxin repressor



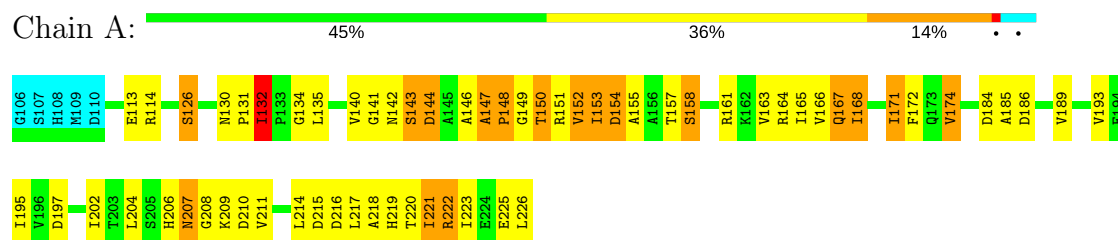
4.2.12 Score per residue for model 12

- Molecule 1: Diphtheria toxin repressor



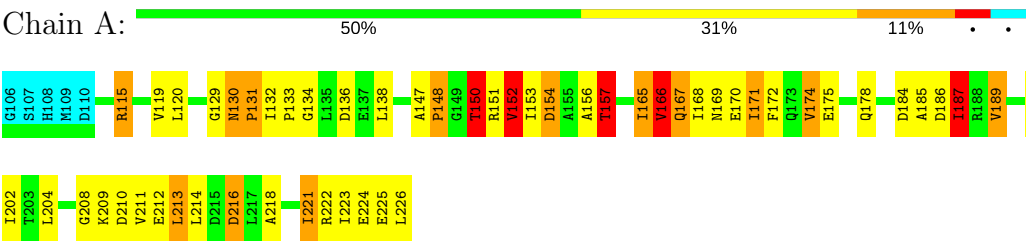
4.2.13 Score per residue for model 13

- Molecule 1: Diphtheria toxin repressor



4.2.14 Score per residue for model 14

● Molecule 1: Diphtheria toxin repressor



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 60 calculated structures, 14 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	1.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	900	907	904	59±12
All	All	12600	12698	12656	820

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:VAL:HG11	1:A:218:ALA:HB1	1.07	1.26	10	2
1:A:163:VAL:HG13	1:A:195:ILE:HD11	0.93	1.38	12	1
1:A:147:ALA:HB1	1:A:148:PRO:HD2	0.83	1.50	10	4
1:A:165:ILE:HD11	1:A:168:ILE:HG12	0.83	1.48	12	1
1:A:135:LEU:O	1:A:137:GLU:N	0.83	2.12	9	1
1:A:152:VAL:HG22	1:A:223:ILE:CD1	0.83	2.03	7	1
1:A:152:VAL:HG22	1:A:221:ILE:HG12	0.81	1.52	6	1
1:A:165:ILE:HA	1:A:223:ILE:HG23	0.81	1.52	14	4
1:A:217:LEU:O	1:A:221:ILE:HD13	0.80	1.75	4	1
1:A:221:ILE:HG22	1:A:223:ILE:HD11	0.80	1.51	4	2
1:A:165:ILE:HD11	1:A:168:ILE:CG1	0.80	2.07	12	2
1:A:150:THR:O	1:A:223:ILE:HD13	0.80	1.77	4	1
1:A:152:VAL:HG13	1:A:202:ILE:HD11	0.80	1.52	11	1
1:A:220:THR:O	1:A:221:ILE:HD12	0.79	1.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:HB2	1:A:223:ILE:HG21	0.78	1.55	13	3
1:A:193:VAL:HG12	1:A:206:HIS:CD2	0.78	2.14	1	5
1:A:132:ILE:N	1:A:187:ILE:HD13	0.75	1.96	14	2
1:A:165:ILE:HG12	1:A:223:ILE:HD12	0.75	1.58	14	1
1:A:112:VAL:HB	1:A:202:ILE:HG22	0.74	1.58	7	1
1:A:132:ILE:HG23	1:A:132:ILE:O	0.74	1.81	12	1
1:A:165:ILE:HD13	1:A:166:VAL:N	0.74	1.98	12	5
1:A:214:LEU:O	1:A:218:ALA:HB3	0.74	1.83	5	3
1:A:151:ARG:CB	1:A:223:ILE:HG21	0.73	2.13	9	1
1:A:132:ILE:N	1:A:133:PRO:CD	0.73	2.50	1	6
1:A:134:GLY:O	1:A:221:ILE:HD11	0.73	1.84	4	2
1:A:135:LEU:CB	1:A:217:LEU:HD22	0.73	2.13	6	1
1:A:137:GLU:O	1:A:168:ILE:HG22	0.73	1.84	7	1
1:A:185:ALA:HB3	1:A:187:ILE:HD11	0.72	1.58	6	2
1:A:151:ARG:O	1:A:153:ILE:HD13	0.72	1.84	3	1
1:A:221:ILE:HB	1:A:223:ILE:HD11	0.72	1.62	1	3
1:A:135:LEU:CB	1:A:217:LEU:HD12	0.72	2.15	11	1
1:A:155:ALA:HB1	1:A:226:LEU:HD21	0.71	1.61	10	1
1:A:153:ILE:HD13	1:A:219:HIS:O	0.71	1.86	11	2
1:A:221:ILE:HG23	1:A:222:ARG:N	0.71	2.00	7	1
1:A:150:THR:O	1:A:153:ILE:HG22	0.71	1.86	14	1
1:A:138:LEU:HD13	1:A:139:GLY:N	0.71	2.01	7	1
1:A:150:THR:O	1:A:153:ILE:HD11	0.70	1.86	3	1
1:A:195:ILE:HD12	1:A:196:VAL:N	0.70	2.02	9	1
1:A:165:ILE:HG23	1:A:165:ILE:O	0.70	1.86	7	2
1:A:151:ARG:N	1:A:155:ALA:HB2	0.69	2.01	4	2
1:A:168:ILE:HG22	1:A:221:ILE:HG23	0.69	1.62	10	1
1:A:204:LEU:HD23	1:A:213:LEU:HD22	0.69	1.63	10	2
1:A:147:ALA:HB1	1:A:148:PRO:CD	0.69	2.17	10	4
1:A:193:VAL:HG12	1:A:206:HIS:CG	0.69	2.22	8	6
1:A:132:ILE:O	1:A:132:ILE:HD13	0.69	1.88	7	2
1:A:167:GLN:O	1:A:168:ILE:HD13	0.69	1.88	11	3
1:A:151:ARG:O	1:A:153:ILE:HG22	0.69	1.87	2	1
1:A:165:ILE:HA	1:A:222:ARG:O	0.68	1.88	7	4
1:A:153:ILE:HG23	1:A:218:ALA:O	0.68	1.88	8	2
1:A:168:ILE:HG22	1:A:221:ILE:HG21	0.68	1.65	9	1
1:A:155:ALA:HB1	1:A:195:ILE:HD13	0.68	1.65	7	1
1:A:156:ALA:HB2	1:A:195:ILE:HG21	0.68	1.66	12	1
1:A:138:LEU:O	1:A:220:THR:HG23	0.68	1.88	10	1
1:A:185:ALA:CB	1:A:187:ILE:HD11	0.68	2.18	14	2
1:A:163:VAL:CG1	1:A:195:ILE:HD11	0.68	2.18	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:VAL:HB	1:A:223:ILE:HG22	0.67	1.65	3	2
1:A:156:ALA:HB2	1:A:202:ILE:HA	0.67	1.66	7	1
1:A:151:ARG:CB	1:A:220:THR:HG22	0.67	2.20	8	1
1:A:139:GLY:O	1:A:140:VAL:HG23	0.67	1.88	1	1
1:A:132:ILE:HD11	1:A:221:ILE:HG21	0.67	1.66	7	1
1:A:131:PRO:O	1:A:132:ILE:HB	0.66	1.89	1	8
1:A:202:ILE:HD13	1:A:203:THR:N	0.66	2.04	5	4
1:A:130:ASN:ND2	1:A:211:VAL:HG22	0.66	2.04	4	1
1:A:154:ASP:O	1:A:157:THR:HG22	0.66	1.91	4	3
1:A:204:LEU:HD12	1:A:213:LEU:HD22	0.65	1.68	14	1
1:A:217:LEU:N	1:A:217:LEU:HD13	0.65	2.04	11	1
1:A:187:ILE:HD12	1:A:187:ILE:N	0.65	2.07	14	1
1:A:147:ALA:O	1:A:149:GLY:N	0.65	2.29	1	2
1:A:129:GLY:O	1:A:130:ASN:O	0.65	2.15	1	5
1:A:131:PRO:O	1:A:132:ILE:CB	0.65	2.45	1	7
1:A:147:ALA:HB3	1:A:148:PRO:HD3	0.65	1.69	11	6
1:A:155:ALA:HA	1:A:226:LEU:HD22	0.65	1.68	5	1
1:A:218:ALA:HA	1:A:221:ILE:HD11	0.65	1.68	3	1
1:A:150:THR:CG2	1:A:155:ALA:HB2	0.64	2.22	1	1
1:A:213:LEU:HD23	1:A:218:ALA:HB2	0.64	1.68	10	2
1:A:182:LEU:HD13	1:A:182:LEU:O	0.64	1.92	2	1
1:A:150:THR:HG23	1:A:223:ILE:HB	0.64	1.69	14	1
1:A:168:ILE:HG22	1:A:221:ILE:CG2	0.63	2.23	9	2
1:A:143:SER:OG	1:A:153:ILE:HG23	0.63	1.93	5	1
1:A:131:PRO:O	1:A:185:ALA:HB1	0.63	1.94	4	1
1:A:220:THR:HG23	1:A:220:THR:O	0.63	1.93	9	1
1:A:164:ARG:O	1:A:223:ILE:HG23	0.63	1.93	13	1
1:A:152:VAL:CG1	1:A:202:ILE:HD11	0.63	2.23	11	2
1:A:130:ASN:CB	1:A:131:PRO:CD	0.63	2.77	4	1
1:A:132:ILE:HD12	1:A:222:ARG:HD2	0.63	1.71	13	1
1:A:151:ARG:H	1:A:155:ALA:HB2	0.62	1.54	13	2
1:A:133:PRO:O	1:A:187:ILE:HG21	0.62	1.93	5	1
1:A:186:ASP:C	1:A:187:ILE:HD13	0.62	2.14	2	1
1:A:134:GLY:HA3	1:A:221:ILE:HG21	0.62	1.71	3	2
1:A:165:ILE:HG22	1:A:191:SER:O	0.62	1.93	7	4
1:A:195:ILE:CG2	1:A:204:LEU:HD23	0.62	2.25	14	1
1:A:131:PRO:HA	1:A:187:ILE:HG21	0.62	1.70	12	1
1:A:152:VAL:HG13	1:A:223:ILE:CG1	0.62	2.24	3	1
1:A:187:ILE:HD13	1:A:222:ARG:NH1	0.62	2.10	7	1
1:A:163:VAL:HG23	1:A:193:VAL:HG23	0.62	1.72	2	1
1:A:167:GLN:C	1:A:168:ILE:HD13	0.62	2.15	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:O	1:A:153:ILE:N	0.62	2.33	2	5
1:A:151:ARG:O	1:A:152:VAL:HG12	0.62	1.95	14	2
1:A:221:ILE:CG2	1:A:223:ILE:HD11	0.62	2.25	14	1
1:A:225:GLU:C	1:A:226:LEU:HD23	0.62	2.15	5	1
1:A:143:SER:CB	1:A:153:ILE:HG23	0.61	2.25	5	1
1:A:155:ALA:CB	1:A:226:LEU:HD21	0.61	2.25	10	1
1:A:165:ILE:CG1	1:A:189:VAL:HG23	0.61	2.26	6	1
1:A:223:ILE:HG22	1:A:224:GLU:H	0.61	1.55	14	1
1:A:152:VAL:HG13	1:A:223:ILE:CD1	0.60	2.25	3	1
1:A:139:GLY:CA	1:A:217:LEU:HD13	0.60	2.26	5	1
1:A:168:ILE:HG21	1:A:220:THR:O	0.60	1.96	7	1
1:A:152:VAL:HG13	1:A:218:ALA:HB1	0.60	1.71	8	1
1:A:150:THR:HG21	1:A:226:LEU:HD22	0.60	1.73	9	1
1:A:149:GLY:O	1:A:163:VAL:HG12	0.60	1.95	7	1
1:A:166:VAL:O	1:A:167:GLN:CB	0.60	2.50	10	3
1:A:135:LEU:HB2	1:A:217:LEU:HD22	0.59	1.73	6	1
1:A:164:ARG:O	1:A:223:ILE:HA	0.59	1.96	3	4
1:A:223:ILE:N	1:A:223:ILE:HD12	0.59	2.11	4	3
1:A:221:ILE:CG2	1:A:222:ARG:N	0.59	2.64	7	2
1:A:155:ALA:CB	1:A:195:ILE:HD13	0.59	2.26	7	1
1:A:139:GLY:O	1:A:140:VAL:CB	0.59	2.49	1	1
1:A:151:ARG:HD2	1:A:153:ILE:HD11	0.59	1.72	8	1
1:A:139:GLY:O	1:A:140:VAL:CG2	0.59	2.50	1	1
1:A:150:THR:HG23	1:A:155:ALA:HB2	0.59	1.75	1	1
1:A:133:PRO:HB2	1:A:182:LEU:HD23	0.59	1.74	8	1
1:A:153:ILE:HD13	1:A:219:HIS:CE1	0.59	2.33	12	1
1:A:145:ALA:O	1:A:146:ALA:HB3	0.59	1.97	7	2
1:A:179:PHE:CZ	1:A:182:LEU:HD12	0.58	2.32	2	1
1:A:152:VAL:HG23	1:A:195:ILE:HG21	0.58	1.75	14	1
1:A:152:VAL:HG23	1:A:223:ILE:HD11	0.58	1.73	5	1
1:A:138:LEU:HD12	1:A:221:ILE:HD11	0.58	1.73	11	1
1:A:149:GLY:HA2	1:A:163:VAL:HB	0.58	1.75	7	1
1:A:151:ARG:HA	1:A:163:VAL:HG11	0.58	1.75	4	1
1:A:138:LEU:HB3	1:A:221:ILE:HG22	0.58	1.75	6	1
1:A:165:ILE:HD13	1:A:223:ILE:HG23	0.58	1.74	3	1
1:A:135:LEU:HD22	1:A:179:PHE:CD2	0.58	2.33	8	1
1:A:187:ILE:HD12	1:A:222:ARG:NH2	0.58	2.13	8	1
1:A:213:LEU:HB3	1:A:218:ALA:HB2	0.58	1.76	6	1
1:A:152:VAL:HG13	1:A:223:ILE:HG12	0.58	1.75	3	1
1:A:213:LEU:HA	1:A:217:LEU:HD23	0.58	1.75	11	1
1:A:174:VAL:HG22	1:A:183:LEU:HD11	0.58	1.74	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:VAL:C	1:A:220:THR:HG21	0.58	2.18	10	1
1:A:202:ILE:HD11	1:A:214:LEU:C	0.58	2.18	14	1
1:A:165:ILE:CD1	1:A:189:VAL:HG12	0.58	2.28	14	1
1:A:221:ILE:HG22	1:A:223:ILE:CD1	0.58	2.29	7	3
1:A:167:GLN:CA	1:A:222:ARG:HB3	0.58	2.29	13	1
1:A:221:ILE:HG23	1:A:222:ARG:H	0.58	1.58	7	1
1:A:135:LEU:HB2	1:A:217:LEU:HD12	0.58	1.73	11	1
1:A:153:ILE:O	1:A:154:ASP:CB	0.58	2.52	13	5
1:A:222:ARG:C	1:A:223:ILE:HD13	0.57	2.20	14	1
1:A:153:ILE:HD13	1:A:153:ILE:N	0.57	2.14	13	1
1:A:163:VAL:HG22	1:A:193:VAL:O	0.57	1.98	5	5
1:A:156:ALA:HB2	1:A:195:ILE:HD11	0.57	1.76	9	1
1:A:135:LEU:HB3	1:A:217:LEU:HD22	0.57	1.75	6	1
1:A:151:ARG:O	1:A:152:VAL:CG2	0.57	2.53	3	1
1:A:163:VAL:CG2	1:A:193:VAL:HG23	0.57	2.29	2	4
1:A:160:PRO:HB3	1:A:226:LEU:HD22	0.57	1.76	1	1
1:A:193:VAL:HG12	1:A:206:HIS:ND1	0.57	2.14	8	2
1:A:128:PHE:O	1:A:211:VAL:HG13	0.57	1.99	8	1
1:A:165:ILE:HD12	1:A:189:VAL:HA	0.57	1.77	9	2
1:A:150:THR:OG1	1:A:155:ALA:N	0.56	2.37	9	1
1:A:165:ILE:HD11	1:A:168:ILE:HG23	0.56	1.76	9	1
1:A:156:ALA:HB2	1:A:195:ILE:CD1	0.56	2.30	2	3
1:A:152:VAL:HG22	1:A:221:ILE:CG1	0.56	2.28	6	1
1:A:132:ILE:HG21	1:A:193:VAL:HG21	0.56	1.77	9	1
1:A:206:HIS:O	1:A:207:ASN:C	0.56	2.43	1	4
1:A:168:ILE:HD13	1:A:187:ILE:CD1	0.56	2.29	10	1
1:A:174:VAL:O	1:A:174:VAL:HG13	0.56	2.00	13	4
1:A:167:GLN:O	1:A:222:ARG:HB3	0.56	2.00	13	3
1:A:138:LEU:HD22	1:A:138:LEU:O	0.56	2.00	7	1
1:A:151:ARG:CB	1:A:163:VAL:HG21	0.56	2.30	4	1
1:A:130:ASN:CB	1:A:131:PRO:HD2	0.56	2.31	6	2
1:A:134:GLY:HA3	1:A:221:ILE:HD13	0.56	1.77	3	1
1:A:167:GLN:O	1:A:222:ARG:CG	0.56	2.53	7	1
1:A:152:VAL:HG11	1:A:221:ILE:HD12	0.56	1.76	12	1
1:A:168:ILE:HD13	1:A:187:ILE:HD12	0.56	1.77	10	1
1:A:174:VAL:HG13	1:A:174:VAL:O	0.56	2.01	11	4
1:A:133:PRO:HG3	1:A:211:VAL:HG11	0.56	1.76	8	1
1:A:166:VAL:O	1:A:189:VAL:HG22	0.56	1.99	6	1
1:A:165:ILE:HG23	1:A:222:ARG:HG3	0.56	1.77	13	2
1:A:152:VAL:HG21	1:A:218:ALA:HB1	0.56	1.77	13	1
1:A:163:VAL:HB	1:A:223:ILE:O	0.55	2.00	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:VAL:O	1:A:154:ASP:N	0.55	2.39	2	4
1:A:135:LEU:HB3	1:A:217:LEU:HD12	0.55	1.77	11	1
1:A:156:ALA:O	1:A:157:THR:HG23	0.55	2.01	14	3
1:A:130:ASN:CB	1:A:131:PRO:HD3	0.55	2.31	12	1
1:A:165:ILE:HD11	1:A:168:ILE:HD11	0.55	1.79	4	1
1:A:147:ALA:HB3	1:A:148:PRO:CD	0.55	2.31	11	6
1:A:132:ILE:N	1:A:133:PRO:HD3	0.55	2.15	1	5
1:A:175:GLU:O	1:A:176:THR:HG23	0.55	2.00	8	2
1:A:150:THR:HG21	1:A:224:GLU:HB2	0.55	1.79	6	1
1:A:120:LEU:HG	1:A:217:LEU:HD21	0.55	1.78	6	1
1:A:152:VAL:CG1	1:A:218:ALA:HB1	0.55	2.32	8	3
1:A:214:LEU:HD23	1:A:214:LEU:N	0.55	2.17	5	1
1:A:149:GLY:O	1:A:153:ILE:HG23	0.55	2.02	4	1
1:A:204:LEU:CD2	1:A:213:LEU:HD22	0.55	2.31	5	2
1:A:152:VAL:CG2	1:A:221:ILE:HG23	0.55	2.32	6	1
1:A:186:ASP:O	1:A:187:ILE:O	0.55	2.25	3	5
1:A:179:PHE:CD1	1:A:182:LEU:HD22	0.54	2.37	8	2
1:A:132:ILE:O	1:A:132:ILE:CG2	0.54	2.53	12	1
1:A:221:ILE:HD11	1:A:223:ILE:HG12	0.54	1.79	6	1
1:A:152:VAL:H	1:A:223:ILE:HD13	0.54	1.61	12	1
1:A:174:VAL:O	1:A:174:VAL:CG1	0.54	2.54	10	1
1:A:187:ILE:HD12	1:A:222:ARG:HH22	0.54	1.61	8	1
1:A:195:ILE:CG2	1:A:204:LEU:HD13	0.54	2.33	5	2
1:A:225:GLU:O	1:A:226:LEU:HD23	0.54	2.03	5	1
1:A:168:ILE:HG13	1:A:187:ILE:HD12	0.54	1.79	1	1
1:A:138:LEU:HD22	1:A:138:LEU:C	0.54	2.23	7	1
1:A:169:ASN:OD1	1:A:187:ILE:HD11	0.54	2.03	9	1
1:A:165:ILE:CG2	1:A:165:ILE:O	0.54	2.56	7	3
1:A:158:SER:O	1:A:226:LEU:HD22	0.53	2.03	11	1
1:A:173:GLN:O	1:A:174:VAL:HG12	0.53	2.03	11	1
1:A:168:ILE:HD12	1:A:169:ASN:N	0.53	2.18	9	1
1:A:187:ILE:HG13	1:A:187:ILE:O	0.53	2.03	1	2
1:A:151:ARG:HB2	1:A:221:ILE:HB	0.53	1.79	11	1
1:A:152:VAL:HG22	1:A:223:ILE:HD13	0.53	1.76	7	1
1:A:153:ILE:HG21	1:A:220:THR:HA	0.53	1.81	9	1
1:A:217:LEU:O	1:A:221:ILE:HD11	0.53	2.04	9	1
1:A:119:VAL:HG13	1:A:120:LEU:N	0.53	2.18	7	1
1:A:132:ILE:O	1:A:168:ILE:HG21	0.53	2.04	12	1
1:A:167:GLN:O	1:A:168:ILE:HB	0.53	2.03	8	2
1:A:155:ALA:HA	1:A:226:LEU:HD23	0.53	1.81	12	1
1:A:168:ILE:CD1	1:A:187:ILE:HD12	0.53	2.32	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:O	1:A:152:VAL:HG22	0.53	2.04	3	1
1:A:152:VAL:HG11	1:A:218:ALA:CB	0.53	2.34	6	2
1:A:186:ASP:O	1:A:187:ILE:C	0.53	2.47	2	3
1:A:131:PRO:CB	1:A:187:ILE:HA	0.53	2.34	1	2
1:A:195:ILE:HD12	1:A:204:LEU:HD22	0.53	1.81	7	1
1:A:138:LEU:O	1:A:140:VAL:N	0.53	2.42	1	2
1:A:150:THR:C	1:A:155:ALA:HB2	0.53	2.24	9	1
1:A:223:ILE:HD12	1:A:223:ILE:N	0.52	2.19	12	3
1:A:151:ARG:HB3	1:A:220:THR:HG22	0.52	1.80	8	1
1:A:149:GLY:O	1:A:226:LEU:N	0.52	2.43	7	1
1:A:138:LEU:HD22	1:A:216:ASP:O	0.52	2.05	14	2
1:A:167:GLN:O	1:A:168:ILE:CB	0.52	2.58	8	3
1:A:146:ALA:HB3	1:A:222:ARG:NE	0.52	2.18	9	1
1:A:167:GLN:CB	1:A:222:ARG:HA	0.52	2.34	8	2
1:A:225:GLU:C	1:A:226:LEU:HD12	0.52	2.23	11	1
1:A:138:LEU:HD22	1:A:217:LEU:O	0.52	2.04	1	1
1:A:186:ASP:O	1:A:187:ILE:HG23	0.52	2.04	14	1
1:A:152:VAL:HG13	1:A:223:ILE:HD13	0.52	1.80	3	1
1:A:148:PRO:O	1:A:224:GLU:HB2	0.52	2.03	7	1
1:A:145:ALA:O	1:A:146:ALA:CB	0.52	2.57	7	2
1:A:189:VAL:HG13	1:A:189:VAL:O	0.52	2.04	7	2
1:A:137:GLU:HG2	1:A:168:ILE:HD11	0.52	1.81	11	1
1:A:174:VAL:HG11	1:A:183:LEU:CD2	0.52	2.35	8	1
1:A:174:VAL:O	1:A:174:VAL:HG22	0.52	2.05	1	2
1:A:152:VAL:CG2	1:A:223:ILE:HD11	0.52	2.35	10	2
1:A:165:ILE:CG1	1:A:223:ILE:HD12	0.52	2.33	14	1
1:A:166:VAL:O	1:A:167:GLN:C	0.52	2.48	5	1
1:A:213:LEU:O	1:A:214:LEU:HD22	0.52	2.04	10	1
1:A:171:ILE:HD11	1:A:189:VAL:HG12	0.52	1.80	8	1
1:A:156:ALA:HB2	1:A:195:ILE:HG12	0.51	1.81	3	1
1:A:138:LEU:HD21	1:A:216:ASP:O	0.51	2.04	1	1
1:A:202:ILE:O	1:A:202:ILE:HG23	0.51	2.06	13	1
1:A:160:PRO:N	1:A:226:LEU:HD13	0.51	2.21	10	1
1:A:151:ARG:C	1:A:152:VAL:HG23	0.51	2.25	6	3
1:A:130:ASN:OD1	1:A:211:VAL:HG22	0.51	2.05	6	1
1:A:166:VAL:HA	1:A:189:VAL:HG13	0.51	1.83	5	1
1:A:221:ILE:HG22	1:A:222:ARG:N	0.51	2.21	11	2
1:A:171:ILE:O	1:A:172:PHE:C	0.51	2.49	1	1
1:A:152:VAL:CB	1:A:218:ALA:HB1	0.51	2.36	1	1
1:A:206:HIS:O	1:A:208:GLY:N	0.51	2.44	12	8
1:A:225:GLU:O	1:A:226:LEU:C	0.51	2.49	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:GLY:HA2	1:A:163:VAL:CB	0.51	2.36	7	1
1:A:166:VAL:HG13	1:A:190:GLY:HA2	0.51	1.83	7	1
1:A:163:VAL:CG2	1:A:194:GLU:HA	0.51	2.36	6	1
1:A:165:ILE:HD12	1:A:189:VAL:HG12	0.50	1.83	14	1
1:A:152:VAL:CG2	1:A:195:ILE:HG21	0.50	2.35	14	1
1:A:130:ASN:O	1:A:185:ALA:HB1	0.50	2.06	12	1
1:A:123:VAL:HG13	1:A:123:VAL:O	0.50	2.06	9	1
1:A:152:VAL:HG23	1:A:223:ILE:CD1	0.50	2.36	5	1
1:A:132:ILE:H	1:A:187:ILE:HG22	0.50	1.65	5	3
1:A:132:ILE:HG23	1:A:165:ILE:CD1	0.50	2.37	3	1
1:A:222:ARG:O	1:A:223:ILE:HD13	0.50	2.06	14	1
1:A:131:PRO:O	1:A:132:ILE:C	0.50	2.49	13	1
1:A:155:ALA:HA	1:A:226:LEU:HD21	0.50	1.82	1	1
1:A:165:ILE:HG23	1:A:190:GLY:H	0.50	1.67	9	3
1:A:152:VAL:HG22	1:A:204:LEU:HD11	0.50	1.82	13	1
1:A:167:GLN:O	1:A:222:ARG:CA	0.50	2.59	7	2
1:A:151:ARG:HG3	1:A:163:VAL:HG21	0.50	1.82	4	1
1:A:130:ASN:HB2	1:A:131:PRO:HD2	0.50	1.83	14	1
1:A:147:ALA:N	1:A:148:PRO:HD2	0.50	2.22	12	2
1:A:135:LEU:HD13	1:A:176:THR:HG21	0.50	1.84	8	1
1:A:165:ILE:HD11	1:A:168:ILE:CD1	0.50	2.37	1	2
1:A:195:ILE:CG1	1:A:196:VAL:N	0.50	2.75	6	6
1:A:226:LEU:HD23	1:A:226:LEU:N	0.50	2.21	2	1
1:A:165:ILE:C	1:A:165:ILE:HD13	0.50	2.27	9	1
1:A:160:PRO:HA	1:A:226:LEU:HD22	0.50	1.83	10	1
1:A:151:ARG:CD	1:A:221:ILE:O	0.50	2.60	1	1
1:A:150:THR:HG21	1:A:155:ALA:HB2	0.50	1.83	12	1
1:A:132:ILE:O	1:A:132:ILE:HG23	0.49	2.07	6	2
1:A:147:ALA:HB1	1:A:225:GLU:CB	0.49	2.37	4	1
1:A:152:VAL:HG21	1:A:218:ALA:HA	0.49	1.84	6	1
1:A:168:ILE:O	1:A:169:ASN:O	0.49	2.30	8	1
1:A:135:LEU:O	1:A:138:LEU:HD12	0.49	2.08	7	1
1:A:175:GLU:O	1:A:176:THR:O	0.49	2.30	7	1
1:A:219:HIS:O	1:A:220:THR:HG23	0.49	2.07	3	1
1:A:150:THR:HG22	1:A:224:GLU:O	0.49	2.06	12	2
1:A:160:PRO:CA	1:A:226:LEU:HD13	0.49	2.38	10	1
1:A:119:VAL:HG22	1:A:120:LEU:H	0.49	1.67	7	1
1:A:132:ILE:HG21	1:A:187:ILE:HG23	0.49	1.84	4	1
1:A:195:ILE:HD11	1:A:202:ILE:HG13	0.49	1.83	3	2
1:A:151:ARG:CG	1:A:220:THR:HA	0.49	2.37	1	1
1:A:168:ILE:O	1:A:168:ILE:HG22	0.49	2.07	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:GLN:N	1:A:222:ARG:CB	0.49	2.75	8	2
1:A:152:VAL:HG12	1:A:202:ILE:HD13	0.49	1.84	13	1
1:A:183:LEU:O	1:A:183:LEU:HD13	0.49	2.08	8	1
1:A:138:LEU:CD2	1:A:216:ASP:O	0.48	2.61	1	1
1:A:151:ARG:NE	1:A:193:VAL:HG21	0.48	2.23	4	1
1:A:213:LEU:HD12	1:A:213:LEU:O	0.48	2.08	12	1
1:A:153:ILE:O	1:A:154:ASP:HB2	0.48	2.07	9	2
1:A:217:LEU:CD1	1:A:217:LEU:N	0.48	2.76	11	1
1:A:165:ILE:O	1:A:165:ILE:CG2	0.48	2.61	1	1
1:A:217:LEU:O	1:A:221:ILE:CG1	0.48	2.60	11	1
1:A:151:ARG:HB2	1:A:220:THR:HG22	0.48	1.85	8	1
1:A:168:ILE:N	1:A:168:ILE:HD13	0.48	2.23	7	1
1:A:147:ALA:N	1:A:148:PRO:CD	0.48	2.77	12	1
1:A:151:ARG:HG2	1:A:219:HIS:O	0.48	2.09	2	1
1:A:165:ILE:HG23	1:A:222:ARG:O	0.48	2.08	3	1
1:A:189:VAL:O	1:A:189:VAL:HG13	0.48	2.08	6	1
1:A:219:HIS:HD2	1:A:220:THR:HG23	0.48	1.69	7	1
1:A:165:ILE:HD11	1:A:168:ILE:HD13	0.48	1.85	1	1
1:A:150:THR:CG2	1:A:224:GLU:CB	0.47	2.92	6	1
1:A:186:ASP:O	1:A:187:ILE:HG13	0.47	2.08	7	1
1:A:165:ILE:CA	1:A:223:ILE:HG23	0.47	2.34	14	2
1:A:165:ILE:O	1:A:166:VAL:HG13	0.47	2.10	8	1
1:A:132:ILE:HD11	1:A:189:VAL:N	0.47	2.23	13	1
1:A:168:ILE:HD12	1:A:221:ILE:HA	0.47	1.85	8	1
1:A:221:ILE:O	1:A:223:ILE:HD12	0.47	2.10	9	1
1:A:150:THR:HG21	1:A:225:GLU:HA	0.47	1.86	13	1
1:A:167:GLN:O	1:A:222:ARG:CB	0.47	2.63	11	4
1:A:186:ASP:O	1:A:187:ILE:HG12	0.47	2.10	11	1
1:A:112:VAL:CB	1:A:202:ILE:HG22	0.47	2.36	7	1
1:A:165:ILE:O	1:A:165:ILE:HG23	0.47	2.10	1	1
1:A:150:THR:HG21	1:A:224:GLU:CB	0.47	2.39	6	1
1:A:221:ILE:HG13	1:A:223:ILE:HD11	0.47	1.85	6	1
1:A:208:GLY:O	1:A:209:LYS:HG3	0.47	2.09	1	5
1:A:212:GLU:O	1:A:213:LEU:C	0.47	2.53	12	1
1:A:119:VAL:CG1	1:A:120:LEU:N	0.47	2.78	4	1
1:A:118:LYS:HB3	1:A:214:LEU:HD21	0.47	1.86	6	2
1:A:165:ILE:HD13	1:A:222:ARG:O	0.47	2.10	13	1
1:A:138:LEU:O	1:A:220:THR:OG1	0.47	2.31	1	1
1:A:152:VAL:HG22	1:A:221:ILE:HB	0.47	1.87	2	1
1:A:195:ILE:HG22	1:A:204:LEU:HD22	0.47	1.87	5	1
1:A:189:VAL:O	1:A:189:VAL:HG23	0.47	2.09	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:VAL:HG23	1:A:113:GLU:N	0.47	2.25	1	2
1:A:179:PHE:CE1	1:A:217:LEU:HD21	0.47	2.45	8	1
1:A:139:GLY:O	1:A:140:VAL:HB	0.46	2.08	1	1
1:A:222:ARG:C	1:A:223:ILE:HD12	0.46	2.31	8	2
1:A:155:ALA:O	1:A:226:LEU:HD11	0.46	2.10	10	1
1:A:187:ILE:O	1:A:187:ILE:HG13	0.46	2.09	10	2
1:A:214:LEU:HD12	1:A:216:ASP:HB2	0.46	1.87	5	1
1:A:221:ILE:HG22	1:A:223:ILE:CG1	0.46	2.41	7	1
1:A:170:GLU:O	1:A:172:PHE:N	0.46	2.48	8	3
1:A:153:ILE:O	1:A:153:ILE:CG1	0.46	2.64	11	2
1:A:132:ILE:HB	1:A:193:VAL:HG11	0.46	1.87	11	1
1:A:160:PRO:HA	1:A:226:LEU:HD23	0.46	1.86	11	1
1:A:140:VAL:HG12	1:A:141:GLY:N	0.46	2.23	1	1
1:A:187:ILE:HG12	1:A:187:ILE:O	0.46	2.09	2	1
1:A:156:ALA:HB2	1:A:195:ILE:HD12	0.46	1.86	5	1
1:A:150:THR:N	1:A:224:GLU:O	0.46	2.49	7	1
1:A:117:VAL:HG23	1:A:119:VAL:HG23	0.46	1.88	2	1
1:A:150:THR:O	1:A:151:ARG:CB	0.46	2.64	3	1
1:A:129:GLY:O	1:A:130:ASN:CG	0.46	2.54	1	2
1:A:135:LEU:HD23	1:A:182:LEU:CD2	0.46	2.41	12	1
1:A:165:ILE:CD1	1:A:223:ILE:HG23	0.46	2.41	3	1
1:A:152:VAL:HG21	1:A:221:ILE:HG23	0.46	1.87	6	1
1:A:166:VAL:O	1:A:167:GLN:HB2	0.46	2.10	14	1
1:A:132:ILE:O	1:A:151:ARG:NH2	0.46	2.49	11	1
1:A:134:GLY:HA3	1:A:137:GLU:HG2	0.46	1.87	6	1
1:A:165:ILE:HG23	1:A:191:SER:H	0.46	1.71	4	1
1:A:165:ILE:HD13	1:A:167:GLN:H	0.46	1.70	5	1
1:A:149:GLY:HA3	1:A:224:GLU:C	0.46	2.32	7	1
1:A:132:ILE:HD13	1:A:132:ILE:O	0.45	2.09	8	2
1:A:150:THR:HG22	1:A:155:ALA:CA	0.45	2.41	4	1
1:A:135:LEU:HD12	1:A:136:ASP:N	0.45	2.27	12	1
1:A:160:PRO:HA	1:A:226:LEU:HD12	0.45	1.87	9	1
1:A:163:VAL:CG2	1:A:223:ILE:CG2	0.45	2.94	7	1
1:A:202:ILE:HD13	1:A:202:ILE:C	0.45	2.31	8	2
1:A:151:ARG:CG	1:A:163:VAL:HG21	0.45	2.41	9	2
1:A:154:ASP:O	1:A:155:ALA:C	0.45	2.55	7	2
1:A:131:PRO:HA	1:A:187:ILE:CG2	0.45	2.41	12	1
1:A:149:GLY:HA3	1:A:224:GLU:HA	0.45	1.89	5	1
1:A:165:ILE:O	1:A:190:GLY:N	0.45	2.50	7	1
1:A:158:SER:HB3	1:A:226:LEU:HD13	0.45	1.87	11	1
1:A:152:VAL:N	1:A:223:ILE:HD13	0.45	2.26	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LEU:HB3	1:A:221:ILE:HD12	0.45	1.88	14	1
1:A:132:ILE:CG1	1:A:193:VAL:HG11	0.45	2.42	11	1
1:A:147:ALA:HB1	1:A:225:GLU:HB2	0.45	1.89	4	1
1:A:131:PRO:C	1:A:132:ILE:CG1	0.45	2.85	9	2
1:A:167:GLN:HA	1:A:189:VAL:HG11	0.45	1.89	9	1
1:A:151:ARG:O	1:A:153:ILE:CD1	0.45	2.63	3	1
1:A:152:VAL:HG22	1:A:204:LEU:CD1	0.45	2.42	13	1
1:A:149:GLY:CA	1:A:224:GLU:HA	0.45	2.41	5	1
1:A:132:ILE:HD13	1:A:132:ILE:N	0.45	2.27	3	1
1:A:155:ALA:CA	1:A:226:LEU:HD21	0.45	2.41	1	2
1:A:165:ILE:CD1	1:A:168:ILE:HD11	0.45	2.42	4	1
1:A:150:THR:O	1:A:151:ARG:C	0.44	2.54	9	1
1:A:151:ARG:O	1:A:152:VAL:HG23	0.44	2.12	2	1
1:A:149:GLY:CA	1:A:225:GLU:N	0.44	2.81	7	1
1:A:151:ARG:O	1:A:152:VAL:C	0.44	2.55	1	1
1:A:202:ILE:C	1:A:202:ILE:HD13	0.44	2.32	6	2
1:A:186:ASP:O	1:A:187:ILE:CG1	0.44	2.65	3	1
1:A:155:ALA:HA	1:A:226:LEU:HD13	0.44	1.88	2	1
1:A:146:ALA:O	1:A:147:ALA:HB2	0.44	2.13	5	1
1:A:151:ARG:C	1:A:153:ILE:HD13	0.44	2.31	3	1
1:A:112:VAL:HG13	1:A:113:GLU:H	0.44	1.72	8	1
1:A:155:ALA:HB1	1:A:195:ILE:HG21	0.44	1.89	6	1
1:A:152:VAL:HA	1:A:155:ALA:HB3	0.44	1.89	1	1
1:A:187:ILE:HD13	1:A:188:ARG:N	0.44	2.27	12	1
1:A:221:ILE:HG22	1:A:222:ARG:H	0.44	1.72	9	1
1:A:165:ILE:HG22	1:A:191:SER:N	0.44	2.27	11	2
1:A:167:GLN:O	1:A:222:ARG:HA	0.44	2.13	7	1
1:A:183:LEU:HD13	1:A:183:LEU:O	0.44	2.12	7	1
1:A:151:ARG:CB	1:A:221:ILE:HB	0.44	2.43	14	1
1:A:134:GLY:N	1:A:168:ILE:CG2	0.44	2.81	12	1
1:A:164:ARG:O	1:A:223:ILE:CA	0.44	2.66	3	2
1:A:164:ARG:HB2	1:A:224:GLU:HB2	0.44	1.90	3	1
1:A:149:GLY:HA2	1:A:221:ILE:O	0.44	2.13	11	1
1:A:132:ILE:C	1:A:132:ILE:HD13	0.44	2.33	7	1
1:A:169:ASN:HB2	1:A:189:VAL:HG21	0.44	1.89	7	1
1:A:165:ILE:HG23	1:A:191:SER:N	0.44	2.28	4	1
1:A:195:ILE:CD1	1:A:202:ILE:HD11	0.44	2.43	4	1
1:A:221:ILE:HG13	1:A:223:ILE:CD1	0.43	2.44	6	1
1:A:187:ILE:C	1:A:187:ILE:HD13	0.43	2.33	12	1
1:A:173:GLN:O	1:A:174:VAL:HG23	0.43	2.13	8	1
1:A:154:ASP:O	1:A:156:ALA:N	0.43	2.51	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:PRO:HB3	1:A:213:LEU:HD11	0.43	1.90	14	1
1:A:130:ASN:N	1:A:185:ALA:CB	0.43	2.80	13	1
1:A:132:ILE:HG23	1:A:165:ILE:HD12	0.43	1.90	3	1
1:A:149:GLY:HA2	1:A:163:VAL:CA	0.43	2.44	7	1
1:A:151:ARG:HB2	1:A:163:VAL:HG21	0.43	1.90	4	1
1:A:165:ILE:CG1	1:A:168:ILE:HD11	0.43	2.42	4	1
1:A:168:ILE:N	1:A:168:ILE:HD12	0.43	2.27	4	1
1:A:151:ARG:HE	1:A:193:VAL:HG21	0.43	1.72	4	1
1:A:128:PHE:HB3	1:A:182:LEU:HD12	0.43	1.90	12	1
1:A:134:GLY:CA	1:A:221:ILE:HG21	0.43	2.43	13	1
1:A:165:ILE:O	1:A:166:VAL:CG2	0.43	2.66	3	1
1:A:135:LEU:HD23	1:A:179:PHE:CZ	0.43	2.48	10	1
1:A:152:VAL:HG11	1:A:213:LEU:HD22	0.43	1.89	4	1
1:A:168:ILE:HB	1:A:189:VAL:HG21	0.43	1.90	6	1
1:A:165:ILE:HG23	1:A:190:GLY:N	0.43	2.28	12	2
1:A:132:ILE:HD12	1:A:222:ARG:CD	0.43	2.42	13	1
1:A:204:LEU:O	1:A:211:VAL:HG23	0.43	2.14	8	1
1:A:132:ILE:HG22	1:A:133:PRO:HD3	0.43	1.91	7	2
1:A:187:ILE:H	1:A:187:ILE:HD12	0.43	1.73	6	1
1:A:165:ILE:HD11	1:A:168:ILE:CG2	0.43	2.43	9	1
1:A:165:ILE:O	1:A:190:GLY:CA	0.43	2.66	1	2
1:A:133:PRO:CB	1:A:213:LEU:HD11	0.43	2.43	14	1
1:A:187:ILE:CG1	1:A:187:ILE:O	0.43	2.66	2	3
1:A:137:GLU:O	1:A:168:ILE:HD13	0.43	2.14	8	1
1:A:165:ILE:HA	1:A:223:ILE:HA	0.43	1.91	6	1
1:A:151:ARG:HD2	1:A:204:LEU:HD11	0.43	1.91	14	1
1:A:132:ILE:CD1	1:A:193:VAL:HG11	0.43	2.43	9	1
1:A:185:ALA:O	1:A:186:ASP:CB	0.43	2.67	7	2
1:A:150:THR:HG22	1:A:225:GLU:CA	0.43	2.43	5	1
1:A:153:ILE:HD12	1:A:219:HIS:CE1	0.43	2.49	5	1
1:A:213:LEU:HD23	1:A:218:ALA:CB	0.43	2.40	5	1
1:A:160:PRO:HA	1:A:226:LEU:HD13	0.43	1.91	10	1
1:A:132:ILE:CD1	1:A:221:ILE:HG21	0.43	2.41	7	1
1:A:163:VAL:HG23	1:A:193:VAL:CG2	0.43	2.44	4	1
1:A:221:ILE:CG2	1:A:223:ILE:CD1	0.43	2.96	14	1
1:A:131:PRO:HA	1:A:187:ILE:HD12	0.43	1.90	12	1
1:A:151:ARG:CA	1:A:155:ALA:HB2	0.43	2.44	9	1
1:A:132:ILE:HG21	1:A:222:ARG:CZ	0.43	2.44	13	1
1:A:202:ILE:HG23	1:A:214:LEU:HA	0.43	1.90	13	1
1:A:175:GLU:O	1:A:176:THR:CG2	0.43	2.67	7	1
1:A:151:ARG:HB3	1:A:153:ILE:CG2	0.43	2.44	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ALA:CB	1:A:148:PRO:CD	0.43	2.92	8	4
1:A:140:VAL:O	1:A:168:ILE:HG23	0.43	2.14	7	1
1:A:134:GLY:HA3	1:A:137:GLU:CG	0.43	2.44	6	1
1:A:165:ILE:HG12	1:A:189:VAL:HG23	0.43	1.90	6	1
1:A:217:LEU:CD2	1:A:217:LEU:N	0.43	2.82	13	1
1:A:195:ILE:HG23	1:A:204:LEU:HD13	0.43	1.90	5	2
1:A:173:GLN:O	1:A:174:VAL:CG2	0.43	2.66	8	1
1:A:149:GLY:HA3	1:A:224:GLU:N	0.43	2.29	7	1
1:A:131:PRO:O	1:A:132:ILE:CG2	0.43	2.67	1	1
1:A:120:LEU:HD21	1:A:135:LEU:HD11	0.43	1.90	1	1
1:A:219:HIS:C	1:A:219:HIS:CD2	0.42	2.93	6	1
1:A:192:GLU:O	1:A:206:HIS:CE1	0.42	2.72	4	1
1:A:132:ILE:HG21	1:A:193:VAL:CG2	0.42	2.43	9	1
1:A:166:VAL:HG12	1:A:166:VAL:O	0.42	2.14	5	1
1:A:226:LEU:O	1:A:226:LEU:CG	0.42	2.66	5	1
1:A:137:GLU:O	1:A:138:LEU:C	0.42	2.57	11	2
1:A:195:ILE:O	1:A:196:VAL:HG13	0.42	2.14	1	1
1:A:131:PRO:CA	1:A:187:ILE:HD12	0.42	2.43	12	1
1:A:112:VAL:HG13	1:A:113:GLU:N	0.42	2.30	11	2
1:A:195:ILE:HG22	1:A:204:LEU:HD23	0.42	1.89	14	1
1:A:132:ILE:CB	1:A:133:PRO:HD3	0.42	2.43	9	1
1:A:158:SER:HB3	1:A:226:LEU:HD11	0.42	1.91	2	1
1:A:132:ILE:CG2	1:A:133:PRO:HD3	0.42	2.45	11	3
1:A:168:ILE:HD13	1:A:189:VAL:HB	0.42	1.91	4	1
1:A:137:GLU:O	1:A:169:ASN:CB	0.42	2.68	1	1
1:A:132:ILE:H	1:A:187:ILE:HD13	0.42	1.72	6	1
1:A:156:ALA:HB2	1:A:195:ILE:CG2	0.42	2.42	12	1
1:A:131:PRO:C	1:A:133:PRO:HD2	0.42	2.35	3	1
1:A:141:GLY:C	1:A:168:ILE:HD12	0.42	2.35	7	1
1:A:130:ASN:HB3	1:A:131:PRO:CD	0.42	2.44	4	1
1:A:168:ILE:HG22	1:A:169:ASN:N	0.42	2.30	5	1
1:A:131:PRO:O	1:A:132:ILE:CG1	0.42	2.67	3	1
1:A:196:VAL:O	1:A:196:VAL:HG23	0.42	2.15	11	1
1:A:163:VAL:CB	1:A:223:ILE:O	0.42	2.68	6	1
1:A:143:SER:HB3	1:A:153:ILE:HG23	0.42	1.91	5	1
1:A:150:THR:CG2	1:A:151:ARG:N	0.42	2.83	3	1
1:A:163:VAL:CG2	1:A:194:GLU:CA	0.42	2.97	6	1
1:A:131:PRO:CG	1:A:193:VAL:HG12	0.42	2.45	14	1
1:A:153:ILE:HD13	1:A:218:ALA:O	0.42	2.14	14	1
1:A:135:LEU:O	1:A:217:LEU:HG	0.42	2.14	13	1
1:A:151:ARG:HB2	1:A:153:ILE:CD1	0.42	2.45	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:GLU:CG	1:A:168:ILE:HD11	0.42	2.45	11	1
1:A:150:THR:OG1	1:A:151:ARG:N	0.42	2.53	6	1
1:A:163:VAL:CG1	1:A:223:ILE:O	0.42	2.68	6	1
1:A:143:SER:HA	1:A:153:ILE:CG1	0.42	2.45	3	1
1:A:155:ALA:HB3	1:A:195:ILE:HD13	0.41	1.91	6	1
1:A:217:LEU:N	1:A:217:LEU:HD23	0.41	2.30	6	1
1:A:131:PRO:C	1:A:133:PRO:CD	0.41	2.88	3	1
1:A:158:SER:C	1:A:226:LEU:HD22	0.41	2.34	11	1
1:A:221:ILE:CG1	1:A:223:ILE:HD11	0.41	2.45	6	1
1:A:158:SER:O	1:A:226:LEU:HD13	0.41	2.14	11	1
1:A:169:ASN:ND2	1:A:189:VAL:HG11	0.41	2.30	7	1
1:A:150:THR:O	1:A:152:VAL:N	0.41	2.52	4	1
1:A:135:LEU:O	1:A:217:LEU:CG	0.41	2.68	13	1
1:A:158:SER:HB2	1:A:226:LEU:HD12	0.41	1.93	13	1
1:A:149:GLY:HA2	1:A:222:ARG:HA	0.41	1.91	11	1
1:A:149:GLY:HA3	1:A:225:GLU:N	0.41	2.30	7	1
1:A:151:ARG:NH1	1:A:152:VAL:HG13	0.41	2.30	9	1
1:A:151:ARG:C	1:A:152:VAL:CG2	0.41	2.89	2	1
1:A:213:LEU:CA	1:A:217:LEU:HD23	0.41	2.44	11	1
1:A:152:VAL:HB	1:A:218:ALA:HB1	0.41	1.90	1	1
1:A:151:ARG:O	1:A:152:VAL:CG1	0.41	2.67	11	2
1:A:135:LEU:HD22	1:A:179:PHE:CG	0.41	2.50	8	1
1:A:195:ILE:HD12	1:A:196:VAL:H	0.41	1.74	4	1
1:A:155:ALA:C	1:A:226:LEU:HD21	0.41	2.36	1	1
1:A:155:ALA:HA	1:A:226:LEU:HD11	0.41	1.92	11	1
1:A:130:ASN:OD1	1:A:211:VAL:HG13	0.41	2.15	7	1
1:A:138:LEU:HB2	1:A:220:THR:HG23	0.41	1.92	6	1
1:A:140:VAL:HG13	1:A:141:GLY:N	0.41	2.31	13	1
1:A:164:ARG:H	1:A:224:GLU:CB	0.41	2.28	5	1
1:A:187:ILE:O	1:A:187:ILE:CG1	0.41	2.69	5	1
1:A:226:LEU:O	1:A:226:LEU:HG	0.41	2.16	5	1
1:A:131:PRO:O	1:A:132:ILE:HG12	0.41	2.15	3	1
1:A:167:GLN:H	1:A:222:ARG:CB	0.41	2.28	8	1
1:A:113:GLU:O	1:A:115:ARG:N	0.41	2.53	7	1
1:A:179:PHE:CD1	1:A:179:PHE:C	0.41	2.93	7	1
1:A:163:VAL:CB	1:A:223:ILE:HG22	0.41	2.43	7	1
1:A:223:ILE:N	1:A:223:ILE:CD1	0.41	2.79	4	1
1:A:187:ILE:N	1:A:187:ILE:HD12	0.41	2.31	6	1
1:A:151:ARG:O	1:A:218:ALA:HB1	0.41	2.15	14	1
1:A:156:ALA:HB2	1:A:195:ILE:HD13	0.41	1.93	2	1
1:A:174:VAL:CG2	1:A:183:LEU:HD21	0.41	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:VAL:HG22	1:A:113:GLU:N	0.41	2.31	8	1
1:A:158:SER:O	1:A:226:LEU:HD11	0.41	2.16	8	1
1:A:150:THR:HB	1:A:224:GLU:HB3	0.41	1.92	6	1
1:A:219:HIS:CD2	1:A:220:THR:HG22	0.41	2.51	6	1
1:A:138:LEU:HD12	1:A:139:GLY:N	0.41	2.31	6	1
1:A:168:ILE:HD13	1:A:187:ILE:HG12	0.41	1.93	2	1
1:A:220:THR:C	1:A:221:ILE:HD13	0.41	2.36	8	1
1:A:152:VAL:O	1:A:202:ILE:CD1	0.41	2.69	7	1
1:A:138:LEU:CD2	1:A:217:LEU:O	0.41	2.68	1	1
1:A:151:ARG:HG3	1:A:220:THR:HA	0.41	1.92	1	1
1:A:130:ASN:O	1:A:131:PRO:C	0.40	2.59	14	1
1:A:165:ILE:HG12	1:A:222:ARG:O	0.40	2.16	7	1
1:A:165:ILE:HD12	1:A:189:VAL:CB	0.40	2.46	14	1
1:A:150:THR:HA	1:A:153:ILE:O	0.40	2.17	9	1
1:A:151:ARG:CD	1:A:193:VAL:HG21	0.40	2.46	13	1
1:A:139:GLY:HA3	1:A:217:LEU:HD13	0.40	1.93	5	1
1:A:150:THR:O	1:A:151:ARG:HB2	0.40	2.16	3	1
1:A:153:ILE:O	1:A:153:ILE:HG23	0.40	2.15	10	1
1:A:150:THR:O	1:A:155:ALA:HB2	0.40	2.17	9	1
1:A:132:ILE:CB	1:A:193:VAL:HG11	0.40	2.46	11	1
1:A:134:GLY:CA	1:A:137:GLU:HG2	0.40	2.46	6	1
1:A:151:ARG:HB2	1:A:221:ILE:CG2	0.40	2.47	14	1
1:A:165:ILE:HG23	1:A:222:ARG:CG	0.40	2.44	13	1
1:A:132:ILE:H	1:A:133:PRO:CD	0.40	2.29	11	1
1:A:150:THR:O	1:A:153:ILE:CD1	0.40	2.67	3	1
1:A:174:VAL:CG1	1:A:174:VAL:O	0.40	2.69	11	1
1:A:138:LEU:HD21	1:A:216:ASP:C	0.40	2.36	4	1
1:A:112:VAL:HB	1:A:202:ILE:HD12	0.40	1.93	1	1
1:A:151:ARG:HD3	1:A:221:ILE:O	0.40	2.16	1	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	115/121 (95%)	68±4 (59±4%)	29±4 (25±4%)	18±3 (16±3%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1610/1694 (95%)	957 (59%)	402 (25%)	251 (16%)	0 4

All 66 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	174	VAL	14
1	A	187	ILE	13
1	A	154	ASP	11
1	A	132	ILE	11
1	A	207	ASN	10
1	A	213	LEU	10
1	A	148	PRO	9
1	A	168	ILE	9
1	A	130	ASN	9
1	A	167	GLN	8
1	A	169	ASN	7
1	A	140	VAL	7
1	A	157	THR	7
1	A	152	VAL	7
1	A	166	VAL	6
1	A	153	ILE	5
1	A	147	ALA	5
1	A	172	PHE	5
1	A	171	ILE	5
1	A	170	GLU	4
1	A	146	ALA	4
1	A	144	ASP	4
1	A	161	ARG	4
1	A	149	GLY	4
1	A	150	THR	3
1	A	151	ARG	3
1	A	139	GLY	3
1	A	127	PRO	3
1	A	128	PHE	3
1	A	120	LEU	3
1	A	138	LEU	3
1	A	145	ALA	2
1	A	114	ARG	2
1	A	155	ALA	2
1	A	220	THR	2
1	A	156	ALA	2

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Mol	Chain	Res	Type	Models (Total)
1	A	209	LYS	2
1	A	208	GLY	2
1	A	143	SER	2
1	A	126	SER	2
1	A	142	ASN	2
1	A	189	VAL	2
1	A	131	PRO	2
1	A	123	VAL	2
1	A	200	GLY	2
1	A	122	ASP	2
1	A	160	PRO	2
1	A	223	ILE	2
1	A	119	VAL	1
1	A	136	ASP	1
1	A	214	LEU	1
1	A	216	ASP	1
1	A	141	GLY	1
1	A	221	ILE	1
1	A	173	GLN	1
1	A	125	ARG	1
1	A	199	ASP	1
1	A	113	GLU	1
1	A	186	ASP	1
1	A	115	ARG	1
1	A	137	GLU	1
1	A	158	SER	1
1	A	116	LEU	1
1	A	176	THR	1
1	A	112	VAL	1
1	A	124	SER	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	101/105 (96%)	80±3 (79±3%)	21±3 (21±3%)	4	32
All	All	1414/1470 (96%)	1114 (79%)	300 (21%)	4	32

All 76 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	184	ASP	12
1	A	132	ILE	12
1	A	210	ASP	11
1	A	165	ILE	10
1	A	223	ILE	10
1	A	171	ILE	10
1	A	216	ASP	9
1	A	211	VAL	9
1	A	154	ASP	8
1	A	214	LEU	7
1	A	195	ILE	7
1	A	221	ILE	7
1	A	113	GLU	7
1	A	183	LEU	7
1	A	137	GLU	7
1	A	188	ARG	6
1	A	168	ILE	6
1	A	226	LEU	6
1	A	152	VAL	6
1	A	150	THR	5
1	A	153	ILE	5
1	A	130	ASN	5
1	A	187	ILE	5
1	A	158	SER	5
1	A	217	LEU	5
1	A	167	GLN	5
1	A	224	GLU	4
1	A	142	ASN	4
1	A	135	LEU	4
1	A	202	ILE	4
1	A	126	SER	4
1	A	222	ARG	4
1	A	119	VAL	3
1	A	209	LYS	3
1	A	177	ASP	3
1	A	143	SER	3
1	A	219	HIS	3
1	A	176	THR	3
1	A	182	LEU	3
1	A	213	LEU	3
1	A	175	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	122	ASP	3
1	A	123	VAL	3
1	A	120	LEU	3
1	A	166	VAL	3
1	A	220	THR	2
1	A	163	VAL	2
1	A	114	ARG	2
1	A	136	ASP	2
1	A	225	GLU	2
1	A	174	VAL	2
1	A	170	GLU	2
1	A	206	HIS	2
1	A	198	ARG	2
1	A	115	ARG	2
1	A	201	HIS	2
1	A	164	ARG	2
1	A	138	LEU	2
1	A	215	ASP	2
1	A	204	LEU	1
1	A	151	ARG	1
1	A	181	GLN	1
1	A	125	ARG	1
1	A	144	ASP	1
1	A	161	ARG	1
1	A	173	GLN	1
1	A	128	PHE	1
1	A	178	GLN	1
1	A	172	PHE	1
1	A	116	LEU	1
1	A	203	THR	1
1	A	212	GLU	1
1	A	157	THR	1
1	A	112	VAL	1
1	A	197	ASP	1
1	A	140	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided